MEMORANDUM

From: Ron Ryan, U.S. EPA, Emission Factor and Inventory Group
Re: Speciation Profiles and Assignment Files Located on EMCH
Date: March 8, 2002

The purpose of this memorandum is to provide instruction on the usage of the speciation profile and conversion factor files as found on CHIEF's Emissions Modeling Clearinghouse (EMCH) website (http://www.epa.gov/ttn/chief/emch/speciation/index.html).

These files have been developed to allow users to estimate the individual and/or "lumped" chemical species required by air quality models from the more aggregated emissions estimates that are usually reported in emissions inventories. Both organic gases and particulate matter emissions estimates, and to a lesser extent SOx and NOx estimates, must be split, or speciated, into more defined compounds in order to be properly modeled for chemical transformations and deposition. These files include the speciation tables needed for all pollutants, although only organic gases and PM2.5 are detailed below as examples.

Generic filenames will be used in this example, as the specific versions of these files may change from time to time. It is always best to ensure that you are using the latest available version of these data as possible.

Speciation of Organic Gases

Emissions of organic gases are typically reported in emission inventories only as aggregate organics, either as Volatile Organic Compounds (VOC) or as Reactive Organic Gases (ROG). These terms are meant to reflect what specific compounds have been included or excluded from the aggregate estimate. Although USEPA defines VOC to exclude both methane and ethane, and the California Air Resources Board (CARB) defines ROG exclude only methane, in practice it is assumed that the VOC estimates reported to EPA's inventories largely represent non-methane organic compounds. Thus, VOC and ROG inventories are essentially synonymous.

The speciation profiles used to split aggregate organic gas estimates into individual compounds are based on total organic gases (TOG), which includes methane and ethane. Therefore, the inventory-reported estimates of either VOC or ROG must be adjusted upward to account for any methane shown in the profiles before those profiles can be properly applied to create the individual compounds.

Our examples below refers to the lumped molecule approach in the Carbon Bond IV (CB-IV) mechanism, where individual compounds with similar reactivity characteristics or carbon bond structures are grouped into a single mechanism species. Look for more information on the speciation mechanisms specific to your chemical transport model in your model's user manual.

The following example assumes an internal combustion turbine engine which fires distillate oil (diesel fuel) [SCC 20200101] and emits 15 tons of VOC and 20 tons of PM-2.5 per year. The calculations below will estimate example annual speciated emissions for both of these pollutants based on the speciation profile and conversion factor files located on the EMCH Speciation website.

Three steps are usually involved in the speciation of either VOC or ROG: assignment of a speciation profile based on SCC, conversion of VOC (or ROG) to total organic gases (TOG), and multiplication of the assigned profile's split factors times the TOG estimate to create emissions estimates for lumped model species. The first step is to identify the appropriate speciation profile to assign to this source category and pollutant. From the SCC-Profile Assignment File, locate the SCC 20200101 and pollutant VOC.

Table 1. SCC-Profile Assignment File

SCC	Pollutant	Profile
…	…	…
20190099	PM2_5	99999
20200101	**VOC**	**1098**
20200101	PM2_5	35602
…	…	…

The combination of SCC 20200101 and pollutant VOC has been assigned a speciation profile of 1098. (The default profile assignment for VOC, CO, NOx, SOx, NH3, and biogenic emissions is profile "0" if the SCC is not found in the Speciation / Pollutant Profile Assignment File.)

For our second step, from the VOC-TOG Conversion Ratios File, locate the SCC 20200101 in the VOC to TOG table.

Table 2. VOC-TOG Conversion Ratios File (VOC to TOG Table)

SCC	Conversion Factor
…	…
20190099	2.00
20200101	**1.12**
20200102	1.17
…	…

On this record, the VOC to TOG conversion factor is found to be 1.12. Using this conversion factor, TOG is calculated as 15 * 1.12 = 16.80 tons per year.

The final step in speciation of VOC emissions is to assign the variables necessary to generate speciated emissions in either molar or mass form using the speciation profiles found in the CBIV Profiles File. Using our example, and locating speciation profile 1098, we will estimate emissions of formaldehyde (model species code FORM in the table). In application, each species would be estimated using these same procedures.

Table 3. CBIV Profiles File

Profile	Pollutant	Species	Split Factor	Divisor	Mass Fraction
…	…	…	…	…	…
1098	TOG	ETH	0.006213904	1	0.1743
1098	**TOG**	**FORM**	**0.005709348**	**1**	**0.17265**
1098	TOG	NR	0.010482527	1	0.1578714
1098	TOG	OLE	0.002893959	1	0.0665372
1098	TOG	PAR	0.014575323	1	0.3234164
1098	TOG	TOL	0.000149776	1	0.00993
1098	TOG	XYL	0.000133326	1	0.008225
1099	TOG	ALD2	0.002175308	1	0.0806833
…	…	…	…	…	…

From the CBIV Profile File, the Split Factor is the numerator and the Divisor is the denominator in the multiplier computed for mole-based speciation. Therefore, in this case, annual moles of formaldehyde are estimated as:

$$\text{Moles}_{\text{FORM,Ann}} = \text{Emiss}_{\text{TOG,Ann}} * (\text{Split Factor} / \text{Divisor})$$

$$\text{Moles}_{\text{FORM,Ann}} = 16.80 \text{ tons/yr} * (0.005709348 / 1)$$

$$\text{Moles}_{\text{FORM,Ann}} = 0.09591705 \text{ moles}$$

The Mass Fraction is the multiplier used in mass-based speciation. Therefore, in this case, annual tons for formaldehyde are estimated as:

$$\text{Emiss}_{\text{FORM,Ann}} = \text{Emiss}_{\text{TOG,Ann}} * \text{Mass Fraction}$$

$$\text{Emiss}_{\text{FORM,Ann}} = 16.80 * 0.17265$$

$$\text{Emiss}_{\text{FORM,Ann}} = 2.90052 \text{ tons FORM/yr}$$

If the divisor is one, the ratio of the mass fraction to the split factor is the average molecular weight for the species in this profile. In this example, the average molecular weight is estimated as 0.17265/0.005709348 or 30.240. (Note: the average MW for a "lumped species" will vary by profile because different relative amounts of individual compounds will comprise the "lumped species" in different profiles. However, the only individual compound lumped into the FORM model species is formaldehyde. Thus, the average MW of FORM in all profiles is the same, and is equal to the actual MW of formaldehyde.)

The CBIV Profile File used above and included on this web page was generated from the TOG profiles contained in the SPECIATE database provided on this web page and a CBIV Model Species Mapping Table. The SPECIATE database provides the mass fractions of the individual organic compounds that comprise TOG for each profile. These individual compounds must then be mapped into the individual (such as FORM, above) and "lumped" species (such as OLE, PAR,etc, above) which make up a particular chemical mechanism's set of model species. Please check documentation for the particular chemical mechanism you are using for information about the Mapping Table needed and its application.

Other Pollutant Speciation

Unlike VOC speciation, other pollutants do not require a step similar to the conversion of VOC to TOG. Instead, the only two steps are assignment of a profile based on SCC, and multiplication of the profile's mass fractions times the PM2.5 mass to create the individual species masses. Using our engine example, we will speciate PM-2.5 to show these two steps.

The first step is to identify the appropriate speciation profile assigned to this source category and pollutant. From the SCC-Profile Assignment File, locate the SCC 20200101 and pollutant PM2_5.

Table 4. SCC-Profile Assignment File

SCC	Pollutant	Profile
…	…	…
20190099	PM2_5	99999
20200101	VOC	1098

20200101	**PM2_5**	**35602**
…	…	…

Using the same table as before, the SCC 20200101 and the pollutant PM2_5 have assigned a speciation profile of 35602. (The default profile assignment for particulate matter emissions is profile "99999" if the SCC is not found in the SCC-Profile Assignment File.)

The second and final step in speciation of PM-2.5 emissions is to assign the variables necessary to generate speciated emissions in mass form only using the speciation profiles found in the Profile File. Unlike the speciation of VOC, particulate matter is not converted to molar values, as the chemistry applied in the air quality models does not currently require it as direct input. Using our example, and locating speciation profile 35602, we will calculate emissions of elemental carbon (model species code PEC in the table). In application, each species would be estimated using these same procedures.

Table 5. Speciation Profile File

Profile	Pollutant	Species	Split Factor	Divisor	Mass Fraction
…	…	…	…	…	…
35601	PM2_5	PSO4	0.0044	1	0.0044
35602	**PM2_5**	**PEC**	**0.7411**	**1**	**0.7411**
35602	PM2_5	PMFINE	0	1	0
35602	PM2_5	PNO3	0.0016	1	0.0016
35602	PM2_5	POA	0.2244	1	0.2244
35602	PM2_5	PSO4	0.0329	1	0.0329
35603	PM2_5	PEC	0.75	1	0.75
…	…	…	…	…	…

The mass fraction is the value used in the mass-based speciation. Therefore, in this case, annual tons for elemental carbon are calculated as:

$$\text{Emiss}_{\text{EC,Ann}} = \text{Emiss}_{\text{PM-2.5,Ann}} * \text{Mass Fraction}$$

$$\text{Emiss}_{\text{EC,Ann}} = 20.00 * 0.7411$$

$$\text{Emiss}_{\text{EC,Ann}} = 14.82 \text{ tons EC/yr}$$